

Problems and Paradoxes in High-dimensional Data

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Outline

- 1 Motivation
- 2 Paradoxes
- 3 Problems
- 4 A practical example
- 5 Some positives
- 6 Questions?

Sources of high-dimensional data

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- **Biotech:** DNA microarrays, proteomics, transcriptomics etc.

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- etc.

Examples

240p image $\sim 100,000$ pixels, 3 color bandwidth $p \approx 300,000$



Paradoxes

Volume of an n-D ball

- What's the volume of a circle with radius r ?

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Volume of p -dimensional ball with radius $r > 0$

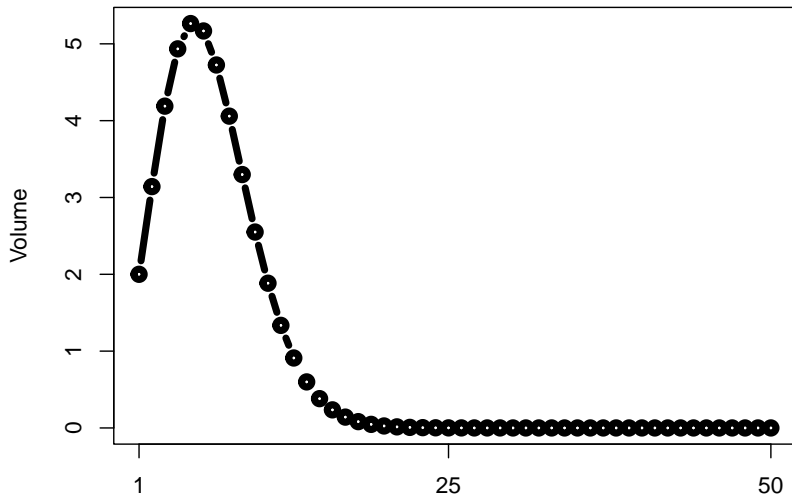
$$V(p; r) = \frac{1}{\Gamma(p/2 + 1)} \pi^{p/2} r^p \quad (1)$$

Does the volume get bigger or smaller as we increase p ?

Or more generally, how does the volume behave?

The volume

The volume



Where is the mass concentrated?

We've noticed that the volume of a p -dimensional ball tends to 0 as p increases, then naturally we might ask:

Where is the mass concentrated?

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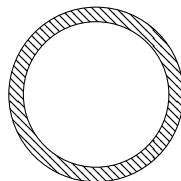
Consider the volume in the crust, i.e. the volume

$$C(p; r) = V(p; r) - V(p; 0.99r) \quad (2)$$

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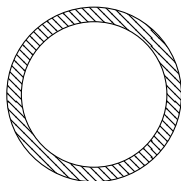
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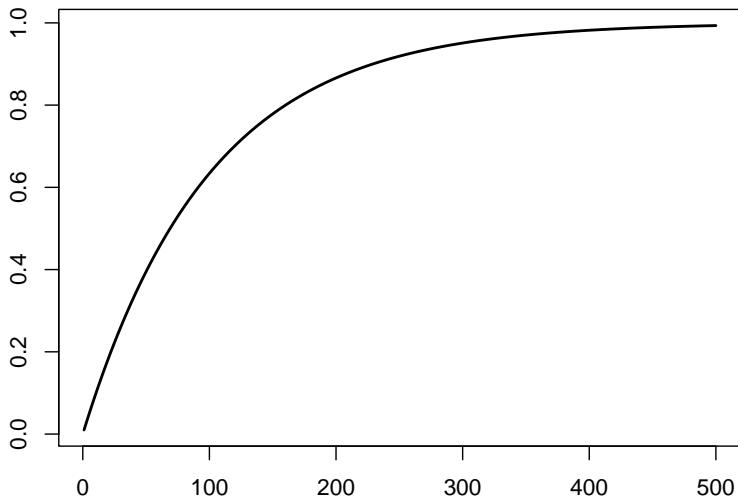
Then the volume in the crust as a fraction of the total volume, i.e.

$$\frac{C(p; r)}{V(p; r)} = 1 - 0.99^p \quad (3)$$



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Recap

- The volume of p -dimensional balls tends to 0
- The crust contains nearly all the mass

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The lesson in all this is, we must be careful with our **geometric intuition** of high-dimensional spaces!

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Paradoxes

There are many more counter-intuitive examples in high-dimensional spaces, to list a few

- Most of the mass of a standard Gaussian is in the tail!
- Rare events may not actually be that rare

Problems

Data get far apart fast

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Suppose we have data uniformly distributed on a 2-D grid, 10-D grid, 100-D grid or 1000-D grid.

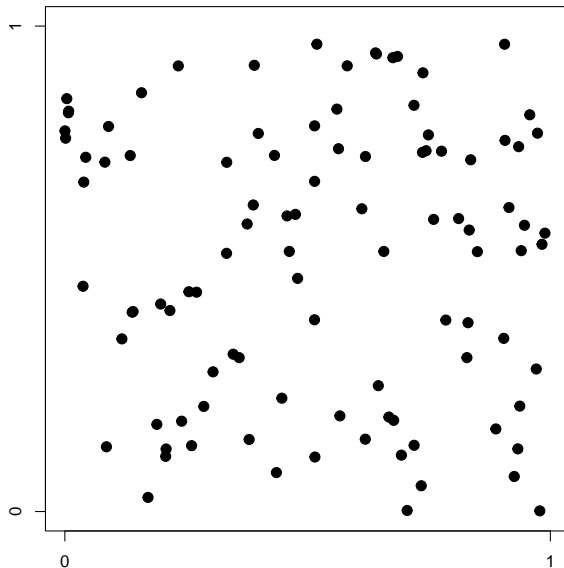
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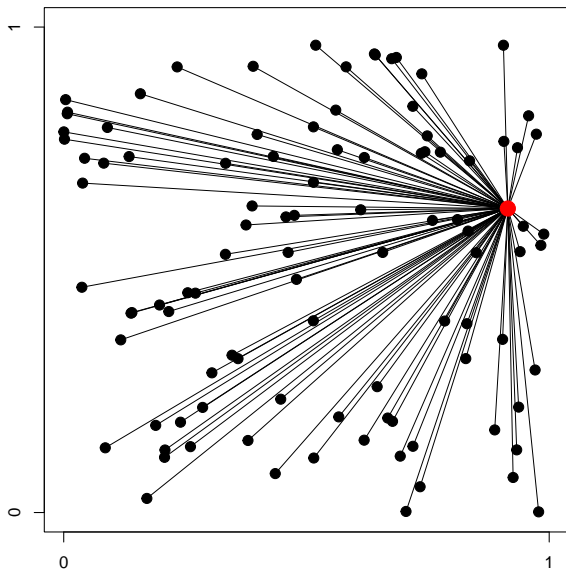
What's the average (euclidean) distance between points?

2D Case

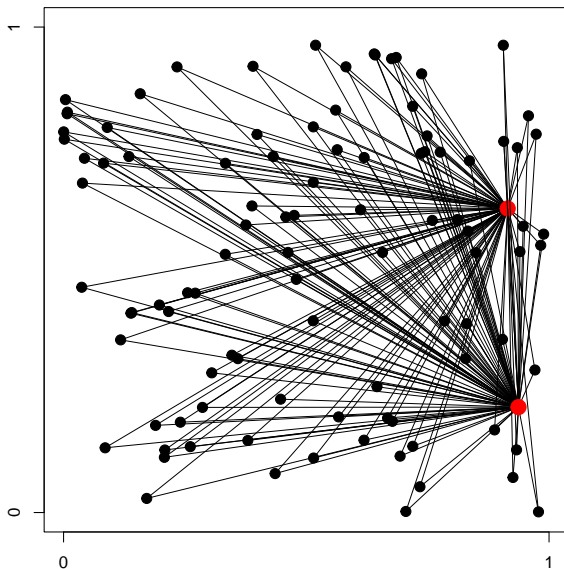
2D Case



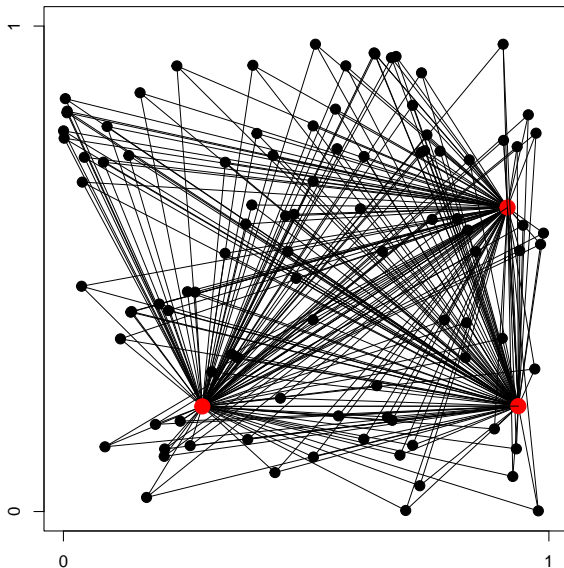
2D Case



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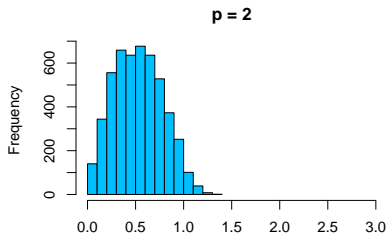


2D Case

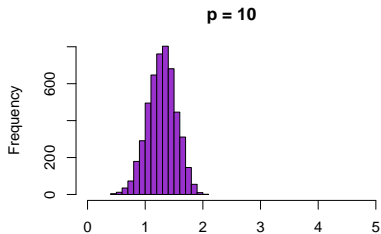
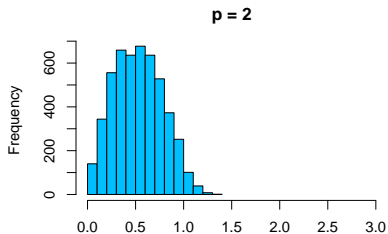


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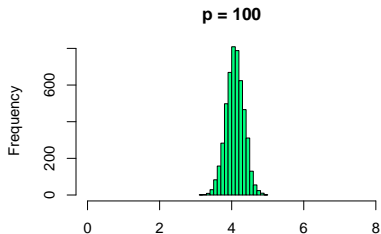
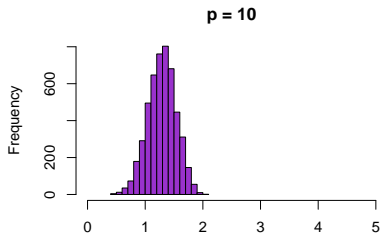
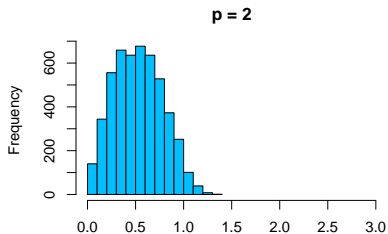
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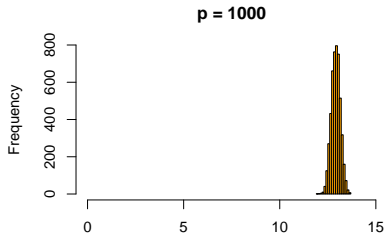
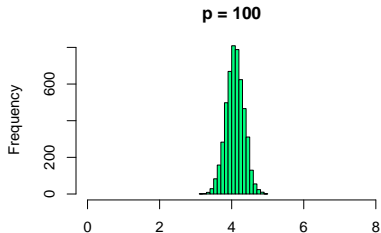
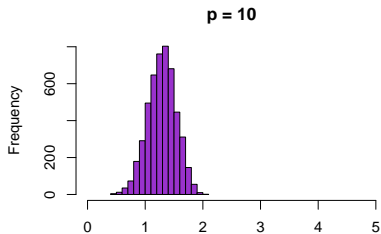
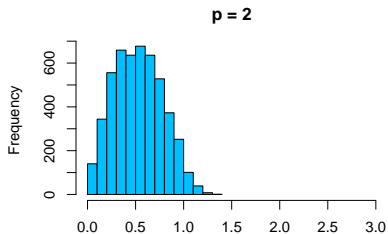
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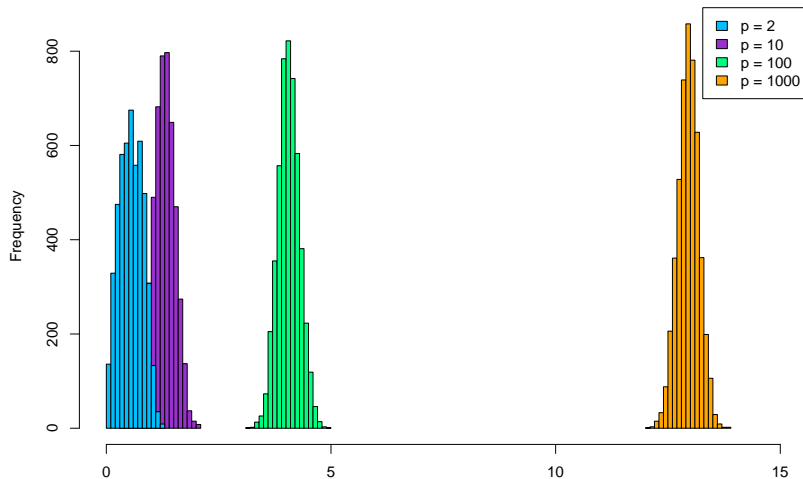


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- The minimal distance between two points increases

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Distances between points

- The minimal distance between two points increases
- All points are a similar distance from the others
- The notion of nearest point vanishes

Some more problems

Some more problems

High-dimensional spaces are immense:

- **Vast**, data points can be isolated in the immensity
- **Small changes add up fast**. Many small fluctuations in different directions can produce a large global fluctuation
- **Computation** suffers

A practical example

PCA

PCA relies on the estimation of the covariance matrix Σ .

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Let's suppose we have some data generated iid from $\text{Normal}(0, I_p)$, where I_p is the $p \times p$ identity.

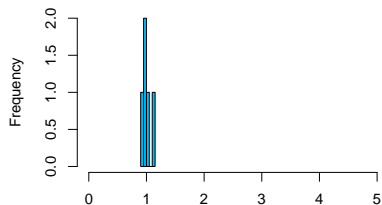
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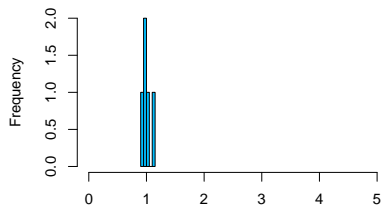
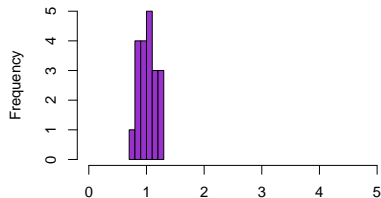
Let's suppose we have some data generated iid from $\text{Normal}(0, I_p)$, where I_p is the $p \times p$ identity.

How well is Σ estimated as p grows?

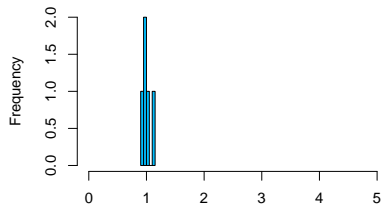
To see how well we're doing we're going to compare the eigenvalues of the estimated covariance matrices to that of the true covariance matrix (I_p), we let $n = 1000$ and let $p = 5, 20, 250, 500$.

$p = 5$

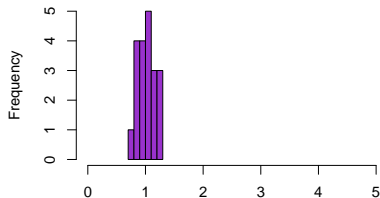


p = 5**p = 20**

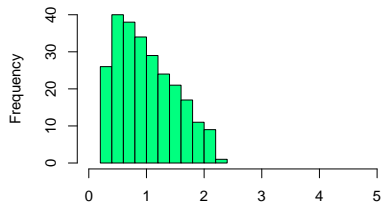
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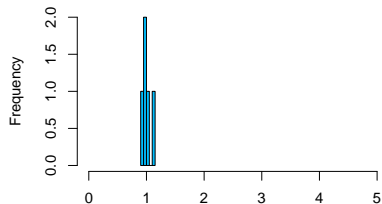
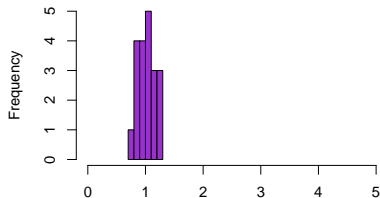
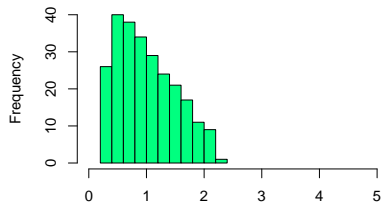
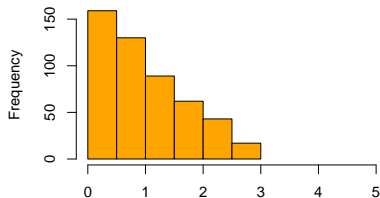


p = 20



p = 250



p = 5**p = 20****p = 250****p = 500**

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In turn, downstream use of the covariance matrix (e.g. in PCA) can lead to spurious results.

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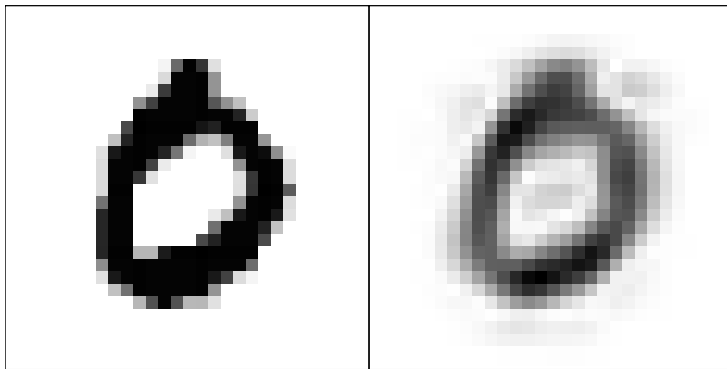
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- etc.

PCA on MNIST

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Reconstructing the MNIST digits from the first 25 PCs



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Methods that can identify relevant structures or **incorporate the knowledge that these spaces are often sparse** generally outperform traditional methods.

Reference I

- [Gir21] Christophe Giraud. *Introduction to High-Dimensional Statistics*. Chapman and Hall/CRC, Aug. 2021.